Classification
(supervised learning)

JJ Valletta

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www.exeter.ac.uk/as/rdp/

Overview

- The classification task

- k-nearest neighbour (kNN)

- Decision trees

- Random forests

- Support vector machines (SVM)

- Over/under-fitting a predictive model

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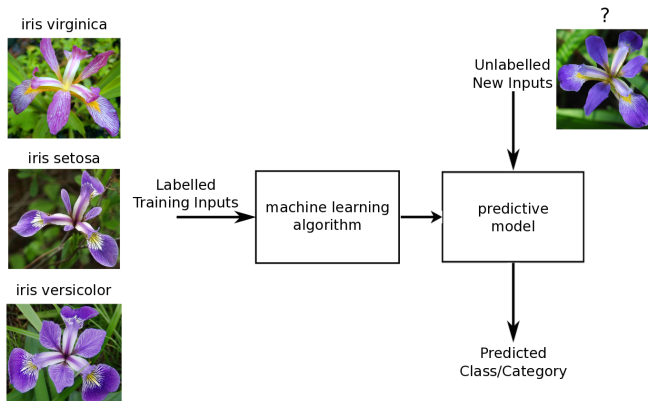
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Classification

Definition

Assigning a set of new observations to a predefined category/class, using a predictive model trained on observations whose category/class is known

iris virginica

iris setosa

iris versicolor

Labelled Training Inputs

machine learning algorithm

Unlabelled New Inputs

?

predictive model

Predicted Class/Category

Note: Better data/features will almost always beat better algorithms

Where are classifiers used?

Medical imaging: is tumour benign or cancerous

Gene expression: use "signature" to classify patient as having (or not) a condition

Computer vision: detect and track a moving object
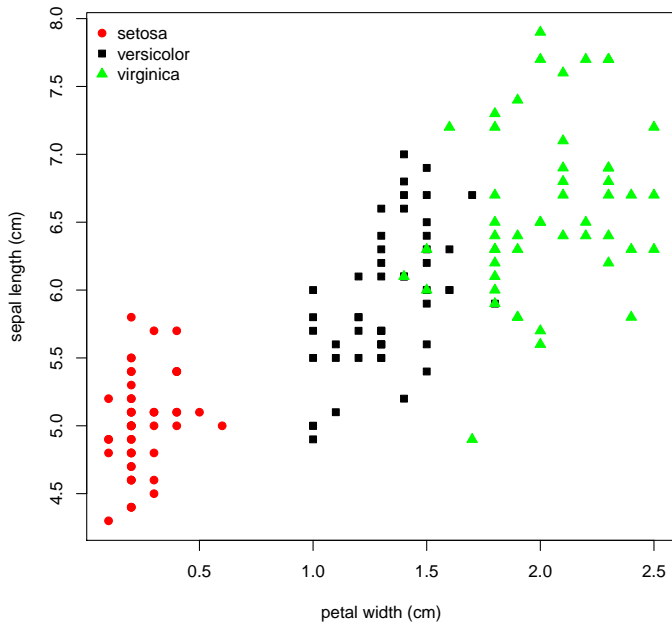
Biogeography: classify land cover using remote sensing imagery

Speech recognition: translate audio signals into written text

Biometric authentication: identify a person using some personal characteristic e.g fingerprint or DNA

Epidemiology: given a set of risk factors what is the chance of patient suffering from a certain condition

Iris dataset

k-nearest neighbour (kNN)

```
library(class)
fit <- knn(train, test, cl, k)
# train - training dataset (matrix or data frame)
# test - testing dataset (matrix or data frame)
# cl - corresponding label of the training dataset (factor)
# k - number of neighbours
```

1. Calculate distance between test point and every training data point

2. Find the k training points closest to test point

3. Assign test point the majority vote of their class label

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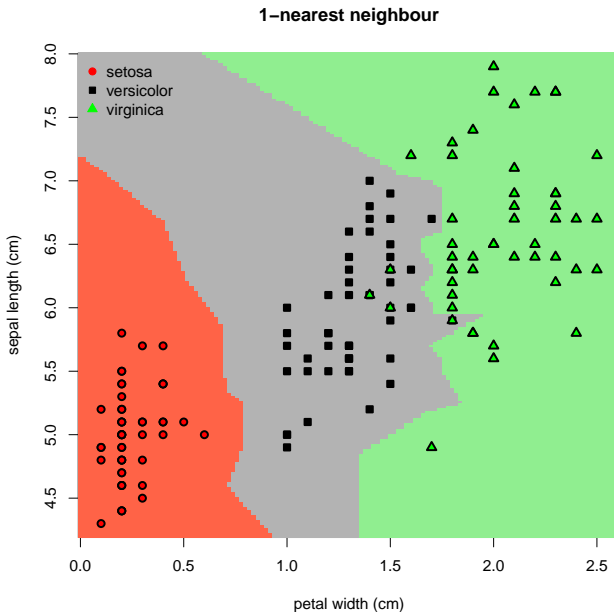
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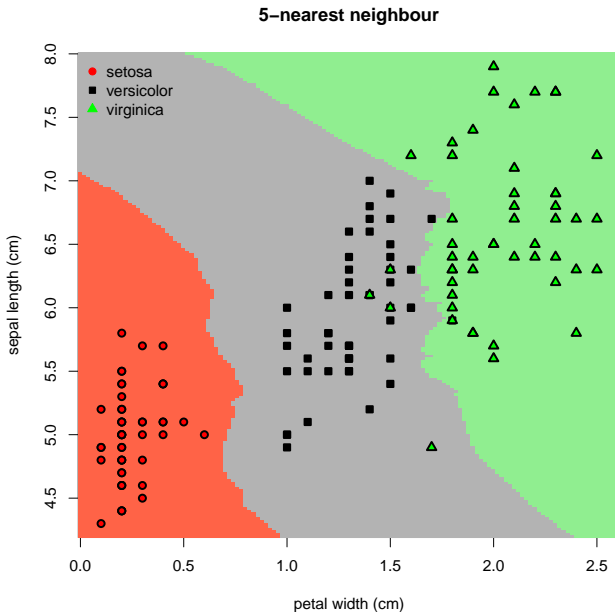
① Calculate distance between test point and every training data point

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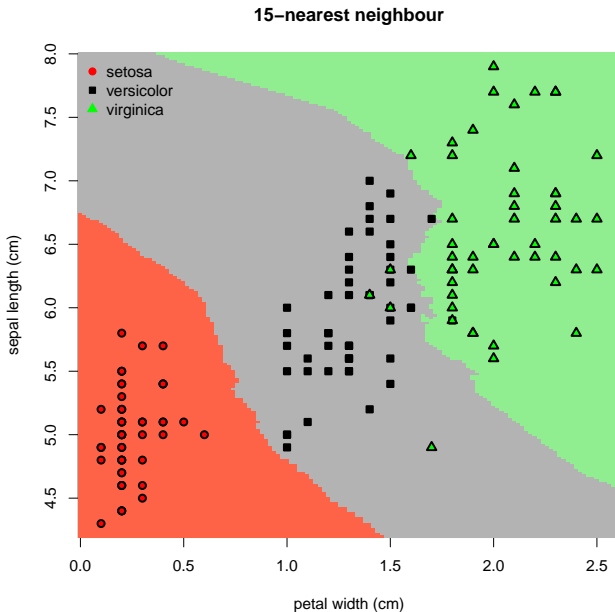
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k-nearest neighbour

1–nearest neighbour

k-nearest neighbour

5–nearest neighbour

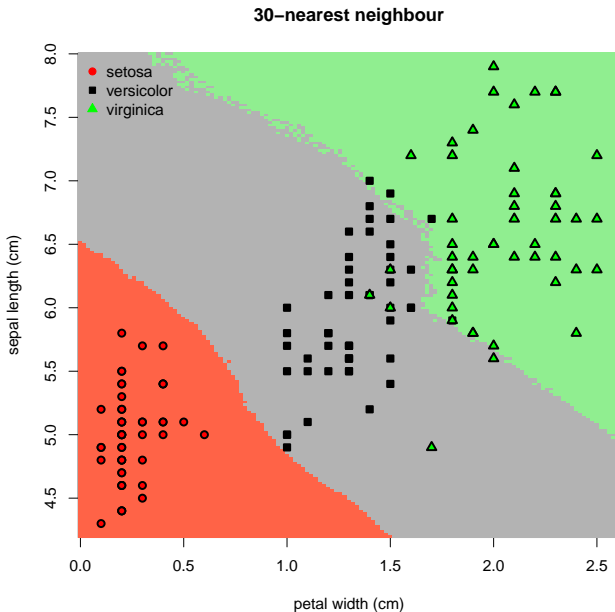# k-nearest neighbour

15–nearest neighbour

k-nearest neighbour

k-nearest neighbour

Pros

- Simple and intuitive
- Works for multi-class problems
- Non-linear decision boundaries
- k easily tuned by cross-validation

Cons

- Can be computationally expensive as for every test point distance to every training data points needs to be computed (the model is actually the whole training dataset)
- Defining nearest by a distance metric can be ambiguous (for e.g when you have categorical predictors)

Decision trees

```
library(tree)
fit <- tree(formula, data)
# OR
library(rpart)
fit <- rpart(formula, data)
# formula - an R formula expression e.g y ~ x1+x2
# data - data frame
```

1. Divide data into left-right (yes-no) by an axis parallel split using *one* predictor

2. The best split is found by maximising information gain/lowering entropy

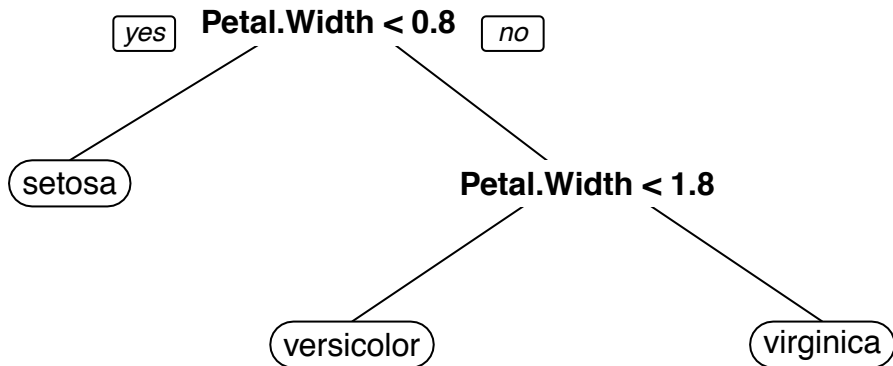3. Repeat 1 to 2 until all data is correctly classified or some stopping rule reached

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Decision trees - The Model

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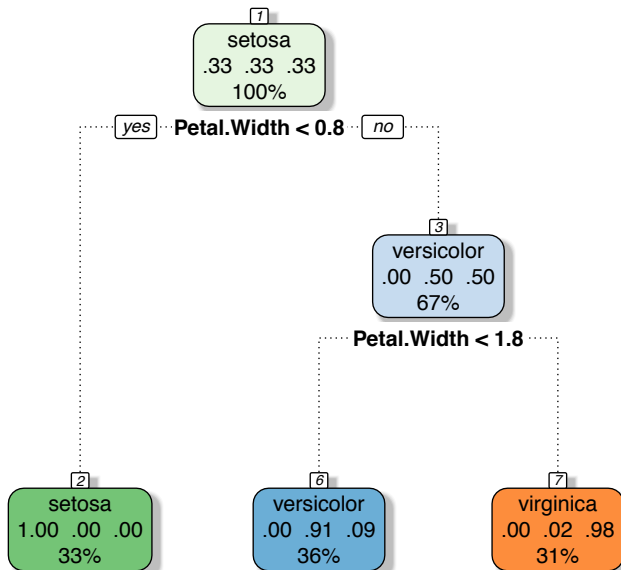
Decision boundaries
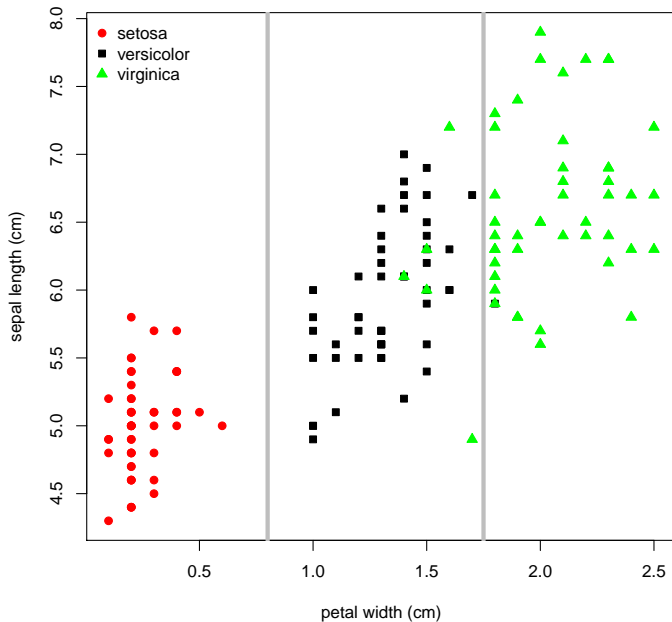
Decision trees

Pros

- Model is very interpretable and can be directly used to generate rules
- Computationaly inexpensive to train and evaluate
- Handle both categorical and continuous data
- Robust to outliers

Cons

- Can easily overfit the data
- Predictive accuracy can be poor
- Small changes to training data may lead to a completely different tree

Random forests

- Decision trees are intuitive but suffer from overfitting which significantly affect their predictive accuracy

- *Pruning*, to "trim" the tree back, help reduce this overfit

- *Ensemble* methods such as Random Forests are a better alternative

- **Rationale**: Instead of one tree, grow a *forest*, where every bushy tree (no pruning) is a bit different, then average predictions over all trees

Random forests

```
library(randomForest)
fit <- randomForest(formula, data, ntree, mtry)
# formula - an R formula expression e.g y ~ x1+x2
# data - data frame
# ntree - number of trees in forest
# mtry - number of predictors randomly sampled as candidates at
    each split (default is sqrt(num of covariates))
```

1. Grow *ntree* bushy trees (no pruning) which are de-correlated from each other

2. Forest randomness is induced by:
   - Bagging (Bootstrap Aggregating i.e each tree is trained on a sample of the data, and only *mtry* sampled with replacement)
   - For every tree, only *mtry* sampled randomly as candidates for the split

3. Average predictions from all *ntree* trees

Random forests

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library(randomForest)
fit <- randomForest(formula, data, ntree, mtry)
# formula - an R formula expression e.g y ~ x1+x2
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1. Grow $ntree$ bushy trees (no pruning) which are de-correlated from each other

2. Forest randomness is induced by:

   - Bagging (Bootstrap AGGregatING), i.e to grow a tree we use a random sample of the data (with replacement) with equal variance

   - The same tree, at each node we randomly sample m predictors as candidates for the split

3. Average predictions from all $ntree$ trees

Random forests

```
library(randomForest)
fit <- randomForest(formula, data, ntree, mtry)
# formula - an R formula expression e.g y ~ x1+x2
# data - data frame
# ntree - number of trees in forest
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Random forests

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library(randomForest)
fit <- randomForest(formula, data, ntree, mtry)
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De-correlated bushy trees in the forest
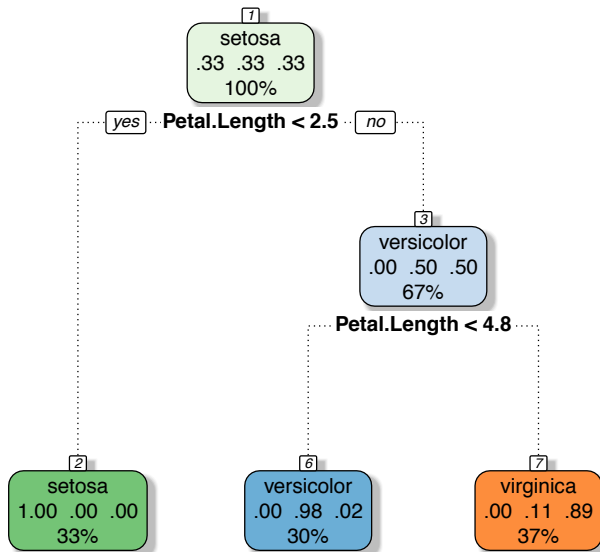
De-correlated bushy trees in the forest
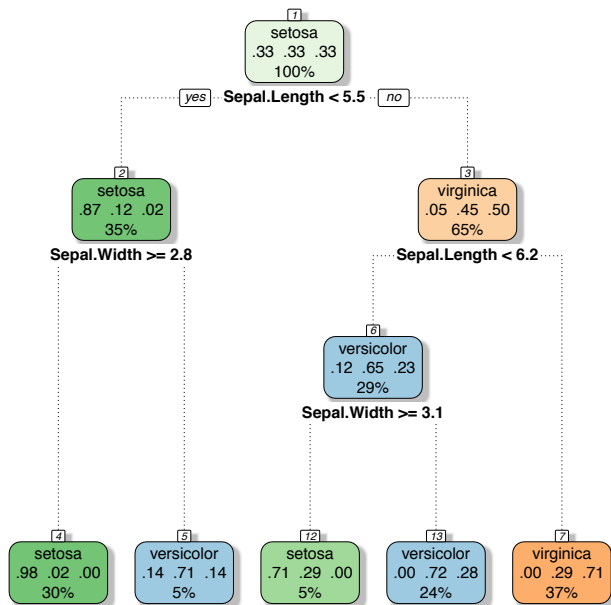
Variable importance (feature selection)

- Cannot visualise decision boundaries (loss of interpretability)
- Predictive accuracy assessed by confusion matrix

	setosa	versicolor	virginica	class.error
setosa	50	0	0	0.00
versicolor	0	47	3	0.06
virginica	0	4	46	0.08

- However, variable importance helps us perform feature selection
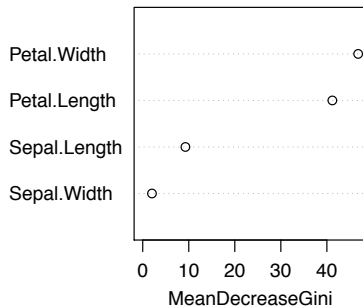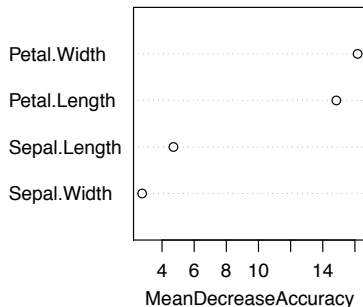
Random forests

Pros

- State-of-the-art predictive accuracy
- Can handle thousands of both categorical and continuous predictors without variable deletion
- Robust to outliers
- Estimates the importance of every predictor
- Out-of-bag error (unbiased estimate of test error for every tree built)
- Can cope with unbalanced datasets by setting class weights

Cons

- Harder to interpret then plain decision trees

Support vector machines (SVM)
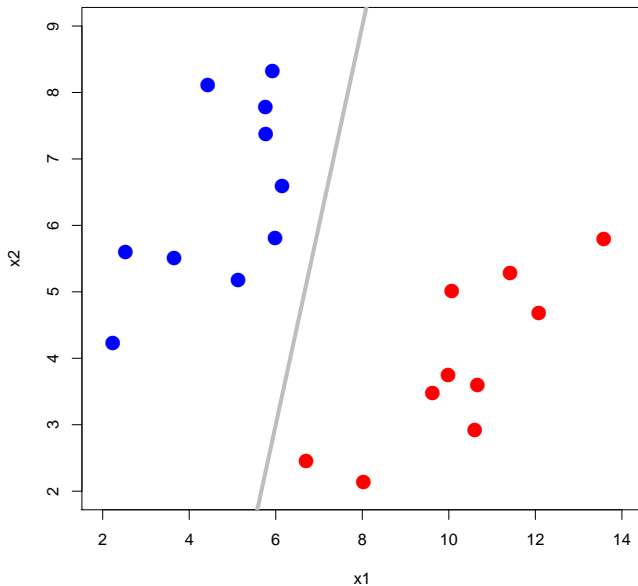
Which is the best separating line?

Support vector machines (SVM)

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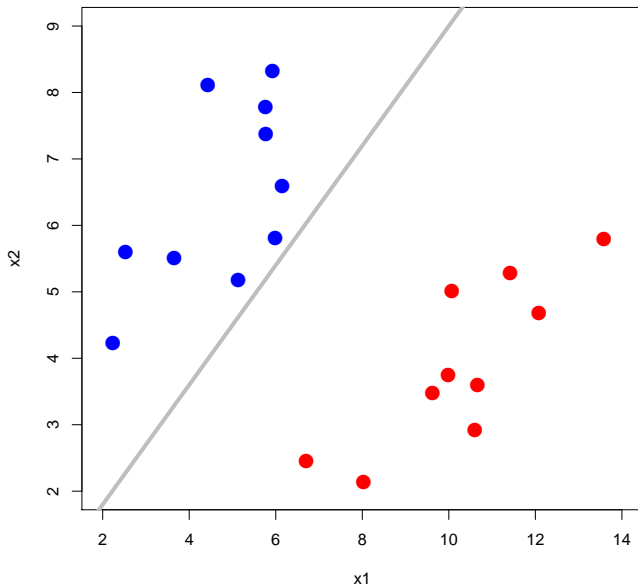
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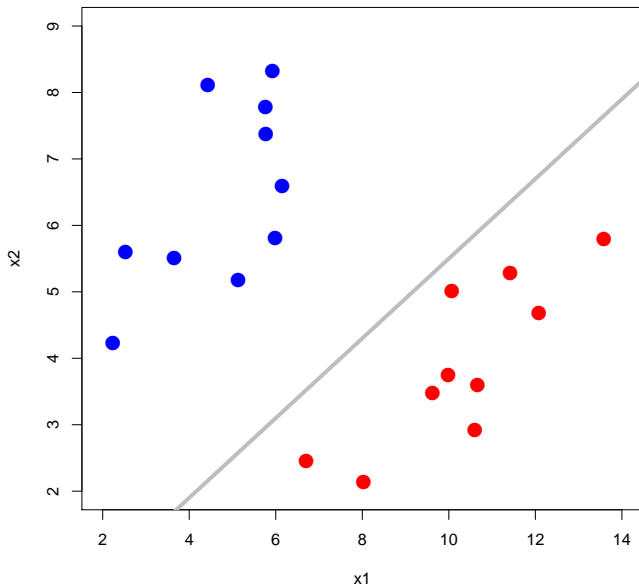
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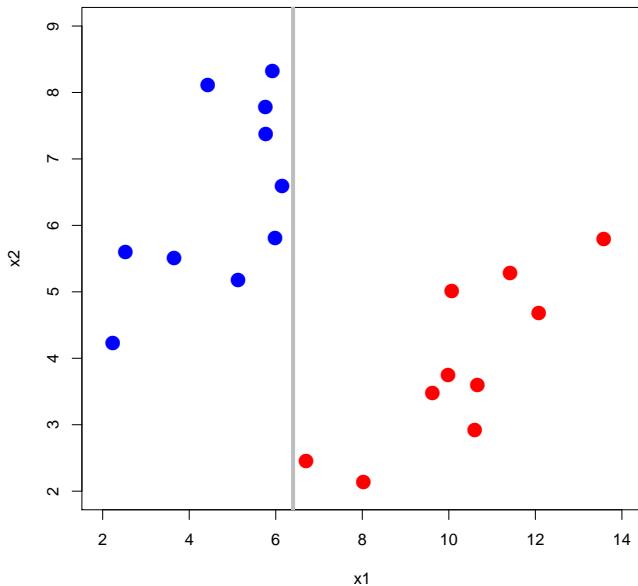
Support vector machines

Rationale: Maximise the *margin*, the distance to separating hyperplane
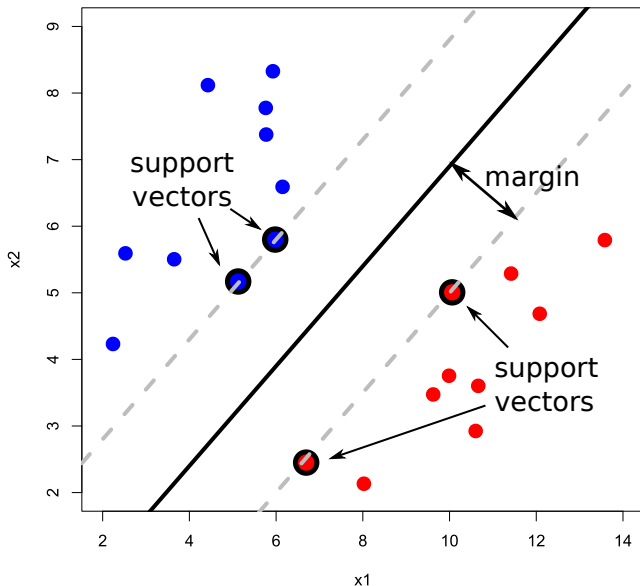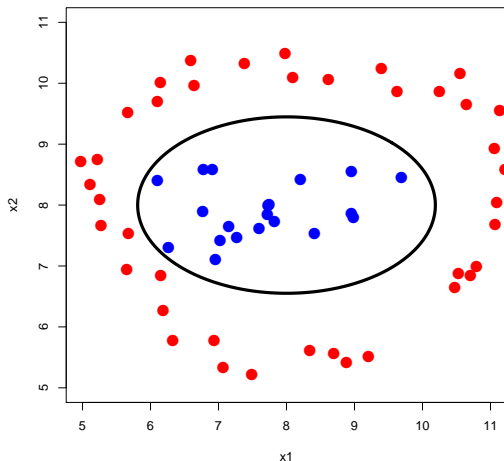
Support vector machines

If it's something weird and it don't look good. Who ya gonna call?
Ghostbusters?
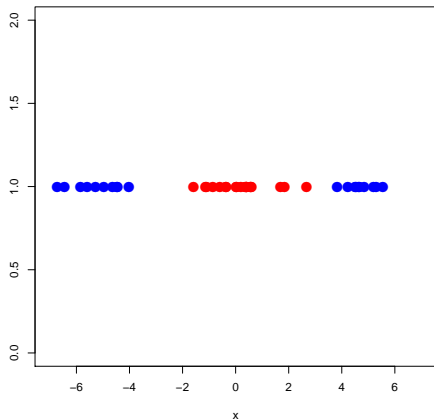*Close*, we need alternate dimensions to make them linearly separable
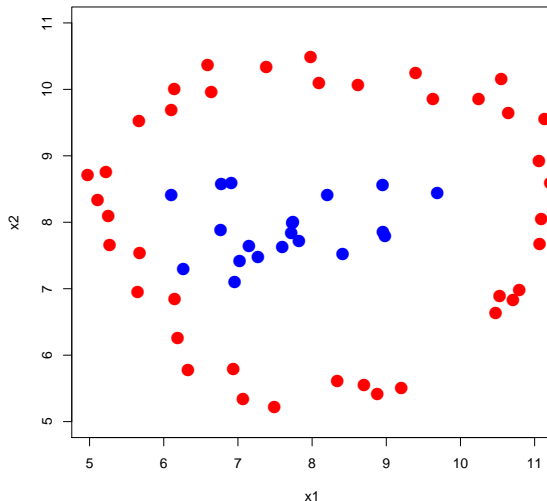
Support vector machines

- Map data to a higher dimensional space where classes are linearly separable (artificially increasing number of predictors)
- $(x_1, \ x_2) \rightarrow (1, \ x_1, \ x_2, \ x_1 x_2, \ x_1^2, \ x_2^2)$
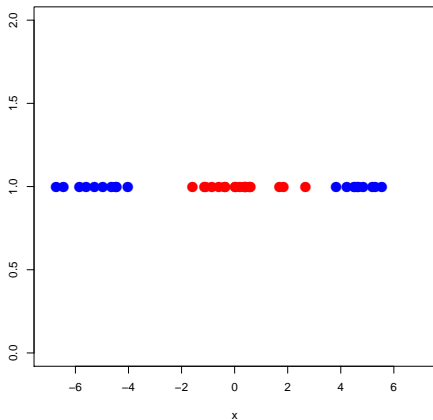- Hyperplane in *new* space is a conic section in *original* space

Support vector machines: Simple example from 1D to 2D
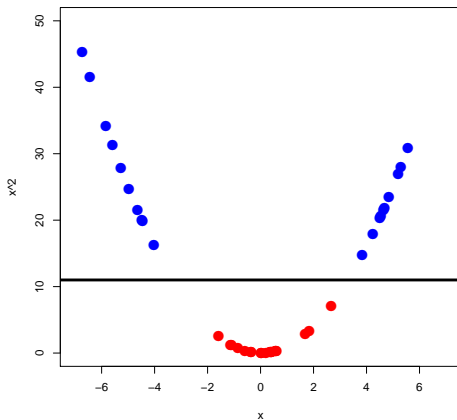

1D (original) data is not linearly separable

Support vector machines: Simple example from 1D to 2D

Support vector machines - The kernel trick

- So our solution is to blow up the dimensions?

- But what about the "curse of dimensionality"?

- Very computationally expensive to work in high dimensions

Support vector machines - The kernel trick

- So our solution is to blow up the dimensions?

- But what about the "curse of dimensionality"?

- Very computationally expensive to work in high dimensions

Kernel trick to the rescue! We work in an *implict* feature space, that is, data is never explicitly computed in higher dimensions.

p.s Kernel methods are mathematically intricate and beyond the scope of this workshop so I will stop here
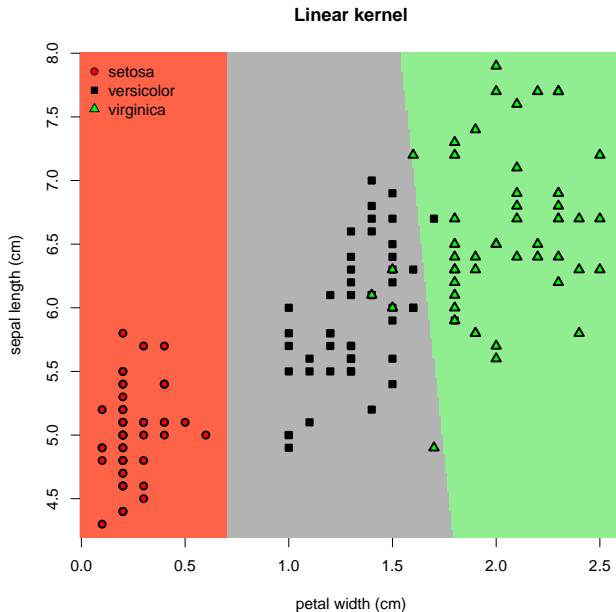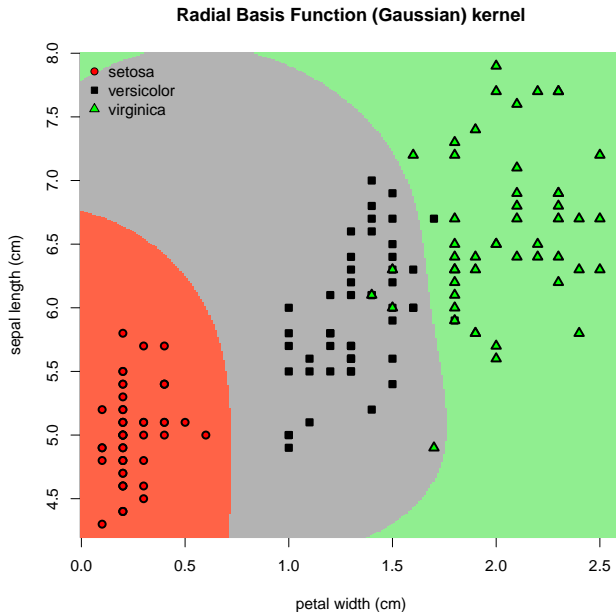
Support vector machines

```r
library(e1071)
fit <- svm(formula, data, type, kernel)
# formula - an R formula expression e.g y ~ x1+x2
# data - data frame
# type - whether the problem is classification or regression
# kernel - the kernel function e.g "linear" or "radial basis"
```

1. Choose carefully a kernel function

2. Run optimiser to find maximum margin

Support vector machines

Support vector machines

Radial Basis Function (Gaussian) kernel

Support vector machines

Pros

- State-of-the-art predictive accuracy
- Less prone to overfitting
- Only need to store the support vectors for the predictive model
- Picking the right kernel gives you flexibility and predictive power
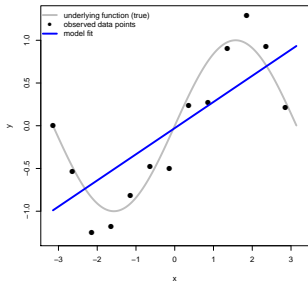- Global optimum guaranteed

Cons

- Unintuitive/a black box
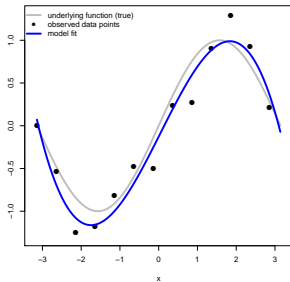- Cannot visualise the feature space

Over/under-fitting (bias-variance tradeoff)

- How well should we fit the training data to get good generalisation?

- Driving training error to zero is not a good idea

- **Bias** caused by a too rigid model leads to *underfitting*

- **Variance** caused by a too flexible model leads to *overfitting*

- **Occam's Razor**, pick the simplest model that explains your data, *parsimony*